EVALUATING BENNU SURFACE COMPOSITIONS USING MIR SPECTRA OF FINE-PARTICULATE ALBEDO-CONSTRAINED MINERAL MIXTURES AND MULTIVARIATE ANALYSIS. L. B. Breitenfeld[1], A. D. Rogers[1] , T. D. Glotch[1] , V. E. Hamilton[2] , P. R. Christensen[3] , and D. S. Lauretta[4], [1]Dept. of Geosciences, Stony Brook University, Stony Brook, NY, laura.breitenfeld@stonybrook.edu, [2]Dept. of Space Science, Southwest Research Institute, Boulder, CO, [3]School of Earth and Space Exploration, Arizona State University, Tempe, AZ, [4]Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ.

Introduction: Detailed assessment of the asteroid Bennu's mineralogy and compositional variability is broadly applicable to the study of carbonaceous near-Earth asteroids and primitive material within our solar system. Among the chondrites, the spectral properties of Bennu are most analogous to those of a CI or CM chondrite [1- 4]. The OSIRIS-REx spacecraft possesses the OSIRIS-REx Thermal Emission Spectrometer (OTES) instrument that observes Bennu in the mid-infrared (MIR) and can be utilized for further refining Bennu's mineralogy [e.g. 4].

There are many factors including composition and particle size that impact MIR spectral properties. Currently available spectral and thermal data from OTES do not yet support a significant fine-particulate component (<60 microns) on Bennu. However, given that OTES spectra cannot be satisfactorily modeled by library spectra consisting entirely of coarse particulates (>90 microns) [5], a further investigation of the contribution of fines is worthwhile. Additionally, it is possible that small regions spectrally dominated by finer-particulate components might be observed using higher resolution data during the upcoming Reconnaissance phase of the mission.

Using linear mixing models [6,7], mineral abundance estimates from fine-particulate surfaces (<60 microns) generally have greatly reduced accuracy compared to coarse-particulate surfaces; however, significant improvements may be possible using multivariate analysis. This is because this alternative approach removes the assumption of linear mixing across all wavelengths. Multivariate analysis requires preparation of a training set covering the relevant compositions and particle sizes. This technique has proven as an effective tool for evaluating compositional abundances using several types of spectroscopy [8-10].

In the event that fine-particulate materials are detected in OTES data, we are preparing a fine-particulate (<50 microns) albedo-constrained library and training set for multivariate analysis. Here we present progress on the development of this training set, some initial assessments of expected model accuracy, and plans for future work. In addition, we note some preliminary spectral trends observed in fine-particulate mineral mixtures that might be relevant to OTES spectra.

Sample Preparation: The mineral species utilized in this work are commonly present within CI and CM chondrites [11-13]. These minerals include antigorite, cronstedtite, saponite, magnetite, pyrrhotite, olivine (Fo40, Fo80, Fo95), calcite, dolomite, ferrihydrite, gypsum, and enstatite. Suitable samples were obtained from several museum collections and dealers or synthesized at Stony Brook. Natural samples were hand-picked for purity and in some cases were centrifuged, acid-washed, or magnetically separated to remove unwanted contaminants. Each was hand crushed or milled to create fine-particulate samples (<50 microns).

Mixtures: This work is ongoing and therefore mixtures are still being made. Cronstedtite-bearing mixtures are not yet available. This precludes immediate application to OTES spectra at this time.

The suite of 13 minerals common in CI and CM chondrites was utilized as end-members within the multivariate analysis models. All samples were darkened using 11 volume% carbon powder [14] to constrain the albedo of the samples to more closely match Bennu albedo.

Using these samples, analog CI and CM meteorite mixtures were made using modal abundances that encompass literature values [4,11,12]. Binary and ternary mineral mixtures were also made. Using binary and ternary mixtures in this project is helpful in two ways.

1. Isolating complex mixing effects for the multivariate model and our understanding.
2. Ensuring every mineral in the model has several data points between 0 and 100 volume%.

This is important, because although narrower model ranges can allow for precise predictions, a restricted model could bias prediction results and would be unable to detect true outliers accurately.

Instrumentation: MIR spectra were acquired in a simulated asteroid environment (SAE). For these measurements, the Planetary and Asteroid Regolith Spectroscopy Environmental Chamber (PARSEC), a custom-built planetary environmental spectroscopy chamber at Stony Brook University, was utilized. PARSEC is coupled to a Nicolet 6700 FTIR spectrometer for emissivity measurements. Before SAE measurements, the chamber was pumped to ~10^{-5} mbar over several hours and subsequently cooled to <-125°C. Blackbody measurements were acquired at 70 and 100°C while samples were heated to 80°C.

Laboratory Spectral Trends: MIR spectra of antigorite, magnetite and binary mixtures of these two components combined are shown in **Figure 1**. As expected, binary mixtures with a higher proportion of antigorite have stronger antigorite features and vice versa. However, in mixtures, some spectral features become obscured by the presence of the other mineral. Regardless of the relative mineral abundances, the binary mixtures share more similarity to each other than to their pure end-members, showing significantly reduced spectral contrast and a change in slope relative to the pure mineral spectra.

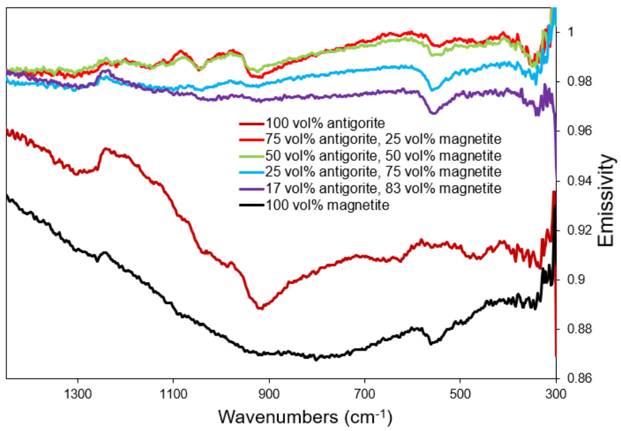

Figure 1. MIR SAE emissivity spectra of antigorite and magnetite end-members with binary mixtures at various volume ratios. All samples were darkened with carbon. The abundance percentages have the carbon removed from the ratio calculations.

Unlike undarkened fine-particulate mineral spectra acquired under ambient conditions, these darkened SAE spectra of fine-grained silicates do not show the characteristic spectral "roll-off" (decrease in emissivity) at high wavenumbers. Ambient measurements of the identical samples similarly lack this spectral "roll-off" indicating the cause is primarily related to presence of the darkening agent. Amorphous carbon, which was used to darken the samples, has an imaginary index of refraction of ~1.5-5 throughout the MIR [15]. We hypothesize that at wavelengths shortward of the Christiansen feature, this high extinction coefficient results in a reduction in the emissivity "roll-off" typically associated with finely particulate silicates.

Multivariate Analysis: MIR spectra of the 13 darkened samples act as endmembers within the multivariate models. In addition to these data, spectra of mixtures were evaluated with partial least squares (PLS1 and PLS2) and least absolute shrinkage and selection operator (Lasso) multivariate analysis [16,17]. PLS1 evaluates one mineral abundance at a time while PLS2 evaluates multiple abundances collectively. Both PLS1 and PLS2 utilize all channels of the spectra while Lasso reduces the number of channels within the model [18].

The accuracy of each model was evaluated using the parameter leave-one-out cross-validated root mean square error (LOO RMSE-CV). This metric is calculated by removing one sample at a time, using a regression model based on the other n-1 samples to predict the n^{th} sample. LOO RMSE-CV gives the best estimate of how the model will perform on unseen data since this error is calculated for predictions that do not rely on itself. LOO RMSE-CV range from 7.2-27.5 volume% for PLS1, 20.9-23.6 volume% for PLS2 and 3.4-26.8 volume% for Lasso models. Model accuracies depend on the type of model, parameters utilized and prediction mineral in question. The creation of these multivariate models is ongoing. As spectra are added to the multivariate models the errors will change.

Ongoing Work: These multivariate models will be applied to spectra of fine-grained CI and CM meteorite samples once the training set is completed. Testing models on "unseen" data (spectra not part of the training set) is an important step to validate the accuracy of the model and for choosing the most appropriate model type (e.g. Lasso, PLS1/2). Last, these models will be applied to regions of Bennu including potential TAG sites.

In addition to the MIR library that has been outlined here, an equivalent VNIR library is also in progress. Comparable multivariate modeling will be applied to OVIRS data.

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